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Nucleonica: Web-based Software Tools for Simulation and Analysis

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ABSTRACT

The authors present a description of a new web-based software portal for simulation and analysis for a wide range of commonly encountered nuclear science applications. Advantages of a web-based approach include availability wherever there is internet access, intuitive user-friendly interface, remote access to high-power computing resources, and continual maintenance, improvement, and addition of tools and techniques common to the nuclear science industry. A description of the nuclear data resources, applications, and tools available at the Nucleonica site is given.

1 INTRODUCTION

As a result of recent developments on issues such as energy security and sustainability, nuclear safety, security, and non-proliferation, and protection of the environment, we are witnessing a resurgence of interest in the nuclear sciences in general. The next generation of reactor energy systems aimed at addressing many of these issues – the so-called *Generation IV* systems – are expected to become available for commercial introduction in the period between 2015 and 2030 or beyond. There is also large range of "non-power" applications of radioisotopes and radiation in a variety of diverse fields such as medicine (e.g. cancer therapy), agriculture (e.g. pest population control), food irradiation (e.g. to increase shelf-life) and in industry (e.g. tracers, radiography, gauging, radiation processing, etc.), where such nuclear skills are also required. In order to support this renewed interest in the nuclear sciences, we will need a nuclear skills renaissance and it is within this context that the Nucleonica nuclear science web portal (www.nucleonica.com) has been developed. With its roots in the traditional paper-based Karlsruhe Nuclide Chart, Nucleonica has grown to become a leading online resource in the nuclear sciences. Nucleonica is particularly suitable for education and training of young scientists, engineers and technicians in the nuclear domain. A variety of our applications enable researchers and specialists to make complex and precise calculations in state-of-the-art fashion.

Due to its advanced IT features, user friendly and intuitive environment, the platform has recently been endorsed by the Sustainable Nuclear Energy Technology Platform (www.snetp.eu): *"Nucleonica plays … an important role in making nuclear education more*

attractive and in building nuclear knowledge for a new generation of engineers and scientists"

The Nucleonica nuclear science portal is an innovative professional and technical resource for knowledge creation and competence building in nuclear science for the worldwide nuclear community. Nucleonica provides a customisable, integrated environment and collaboration platform, using the latest internet "Web 2.0" dynamic technology. A unique feature of Nucleonica is its "electronic knowledge objects", which cover web-based scientific applications, an online wiki and blog as well as forums that enable collaborative research and scientific projects in a worldwide accessible online laboratory.

2 NUCLEAR DATA RESOURCES IN NUCLEONICA

Nucleonica provides users friendly access to the latest reference data from internationally evaluated nuclear data. The Nucleonica database is based on the Joint Evaluated Fission and Fusion (JEFF3.1) radioactive decay datafile [1] which contains decay data on 3852 nuclides in ground and isomeric states. The relational nature of the Nucleonica database allows for fast searching and data retrieval in comparison to the non-relational JEFF3.1 datafile. The Nucleonica database contains information on approximately 93 additional nuclides and their half-lives which are not listed in JEFF3.1 but are present in NUBASE ´03 [2], bringing the total number of nuclides (ground and isomeric states) in the Nucleonica database to 3947. In addition, NUBASE ´03 data on the atomic weights, binding energies, mass excesses, and abundances are included in the Nucleonica database (in the "materials" table).

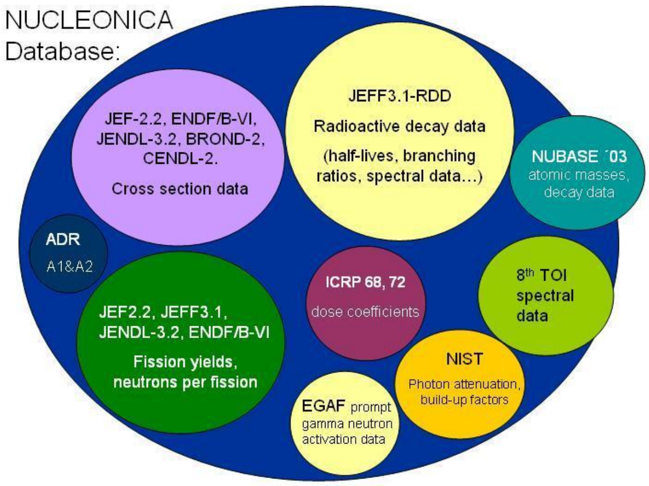

Figure 1: Nuclear data used in the Nucleonica databases

To support the nuclear science applications in Nucleonica, the database is further complemented by a variety of data from other sources (see Fig. 1). Spectral data (energies, emission probabilities etc.) are from JEFF3.1 [1] and the 8th table of isotopes. Photon mass attenuation coefficients and mass energy-absorption coefficients and build-up factors, to model the scattering effects in the shield materials are from NIST. Fission yield data are from the main international datafiles: JEF2.2, JEFF3.1, JENDL-3.2, and ENDF/B-VI. Integral cross section data from JEF Report 14 which contains averaged neutron cross-sections from international datafiles JEF-2.2, ENDF/B-VI, JENDL-3.2, BROND-2, and CENDL-2. Effective dose coefficients for ingestion and inhalation, $e(50)$, are from the ICRP. The A1 and A2 activity and activity exemption limits for packaging and transportation are from the IAEA.

Properties of the elements (densities, melting points, boiling points etc.) and tables of physical constants,conversation factors and radiological limits are from the most recent evaluations. Detailed references to these sources is given in the Nucleonica wiki [2].

The main applications and tools where nuclear data can be found in Nucleonica are the Nuclide Explorer, Universal Nuclide Chart, Fission Yields, Nuclide Datasheets, Nuclear Data Retrieval.

Figure 2: Main nuclear science webpage in Nucleonica Highlighted areas show where to find nuclear data.

3 NUCLEAR SCIENCE APPLICATIONS AND TOOLS

A unique feature of Nucleonica is the wide range of validated web-based nuclear science applications. The core applications include the Mass Activity Converter, Nuclide Mixtures, Decay Engine, Dosimetry and Shielding, Virtual Cloud Chamber, Range and Stopping Power. More advanced applications include webKORIGEN, Neutron Activation, Gamma Spectrum Generator, Gamma Library, Cambio, WESPA (web spectrum analyser) and Scripting. A brief description of these applications follows:

Mass Activity Converter: This is a popular tool for conversion between different physical quantities (e.g. mass, activity, number of atoms, etc.). A particularly useful feature is that in addition to single nuclides, the mass activity calculator can also be applied to nuclide mixtures. These nuclide mixtures can be created with the Nuclide Mixtures application. In addition to the standard conversions (mass, activities, etc.), conversions can also be made using a) external and internal dosimetry quantities, b) the committed effective doses for inhalation and ingestion, c) the amount of heat generated – i.e. isotopic powers through radioactive decay for α, $\alpha+\beta$, $\alpha+\beta+\gamma$.

Nuclide Mixtures: In real life situations, one usually encounters mixtures of nuclides rather than single nuclide. The Nuclide Mixture application allows the user to create and edit nuclide mixtures. Thereafter, these mixtures can be used in the Nucleonica applications. Mixtures can be uploaded and downloaded as xml files. All mixtures can be downloaded into a single xml file. This is useful for backup purposes for sending nuclide mixtures to other users.

Decay Engine: Nucleonica's Decay Engine provides an exact solution to the coupled radioactive decay equations based on the Batemann solution. The Engine can be used for single nuclides and nuclide mixtures and to makle plots of activities, masses etc over a decay time interval. There are two basic modes of operation: a) Time mode - for an initial activity of a given nuclide or mixture, the final activity is calculated after a decay time; b) Date mode - if an activity is known at some time (date), then the activity can be calculated at any other time (date) using a date picker tool. A very useful feature is the Rescale tool. This allows output values to be rescaled to give a desired value. Another useful tool is the slider which allows easy reading of graphical output.

Dosimetry & Shielding: This application has been developed for gamma dose rate and shielding calculations using the point source kernel method. The module allows the user to calculate gamma dose rates from point sources of either single nuclides or composite mixtures. More than 1300 gamma and X-ray emitting nuclides with more than 53,000 gamma and X-rays are available in the Nucleonica database, together with a choice of ten different shield materials. The intuitive interface is ideal for quick and accurate dose calculations such as in health physics or to test more sophisticated Monte Carlo codes. It is ideal for workers in the lab to obtain a rough indication of the dose rate from the radioactive materials they are working with – only a web browser and internet connection required.

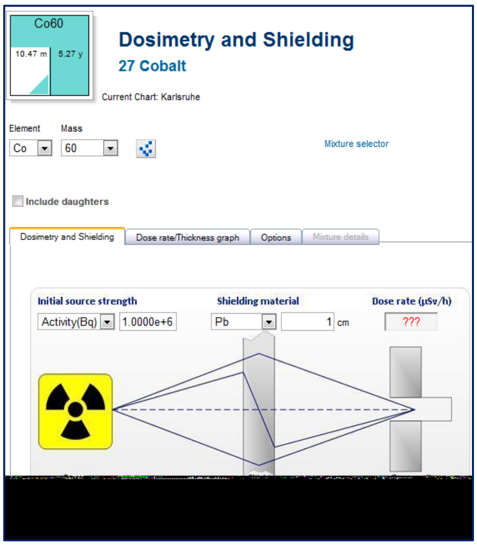

Figure 3: The Dosimetry and Shielding application user interface

Range & Stopping Power: This application provides a user-friendly interface for quick and accurate calculations on the range and stopping powers of charged particles – electrons, positrons, protons, alphas, muons and heavy ions – in matter. Target materials include the natural elements, pre-defined (e.g. tissue) and user-defined compounds. In addition, the user can also select the energy and stopping power units, etc. Range and stopping power results can be displayed in high quality graphs. The underlying calculation engine for stopping power and ranges on heavy ions is based on SRIM (Stopping and Range of Ions in Matter). For electrons, muons, and positrons, a new formulation, has been used. For radiative stopping power the standard ratio is used.

Virtual Cloud Chamber: This is an online interactive simulation tool for investigating the motion of charged particles and photons in different media. The simulation tool, which is based on the Monte Carlo GEANT 4 Engine, has been developed and integrated into

Nucleonica. For the investigations a point source of mono-energetic particles is used. Initially the simulations are restricted to photons, electrons and positrons. To better understand the charged particles emission processes, the various energy loss mechanisms can be "switched-off" in the calculations - otherwise the range of the charged particles would be very small and almost invisible. For photons, there the various energy loss processes - photoelectric effect, Compton scattering, and pair production - can also be switched on/off. In each case, a 1-cm thick lead shield was used.

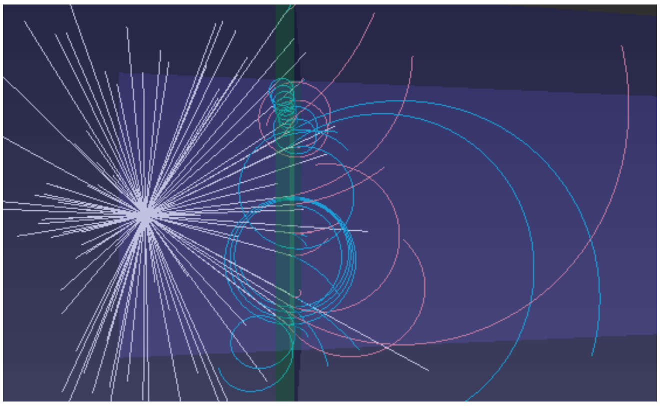

Figure 4: Simulation of high energy gamma photon interaction with a lead shield (green) using Nucleonica'a virtual cloud chamber (positrons: red, electrons: blue; gammas: white). The spiral motion is due to the presence of a magnetic field

webKORIGEN: Nucleonica's webKORIGEN is a very user-friendly and intuitive web-based version of nuclide depletion and burnup code KORIGEN which has been trimmed to three major classes of nuclear plants: Pressurized Water Reactors (PWR), Boiling Water Reactors (BWR), and the European Fast Reactor (EFR). Sub-critical systems can be analysed in the neutron activation mode. There are basically four modes of operation: 1a) Reactor Irradiation (constant power) of fresh nuclear fuel, 1b) Reactor Irradiation (constant flux) allows neutron activation of targets in PWR, BWR, Fast Reactor and Thermal Neutron spectra; 2) Decay of single nuclide and nuclide mixtures; 3) Reactor irradiation (Mode 1) with subsequent period of decay storage; 4) Reactor irradiation and cooling with subsequent reprocessing and waste storage.

Current fuel options are centered on UOX (uranium oxide) and MOX (mixed oxide fuels containing UO_2 and PuO_2). For UOX fuel the initial enrichment is specified, whereas for MOX the plutonium composition and the weight fraction of ^{241}Am/Pu is required together with the fissile plutonium in the initial heavy metal. Target irradiations are restricted to small samples of a single-nuclide material in the irradiation facility. In this way the neutron spectrum in the target is dominated by the reactor facility spectrum.

Gamma Library: The library creation module can be used to create nuclide libraries using the latest internationally evaluated nuclear data. In addition to textformats, some proprietary formats (e.g. GammaVision) are also supported. Such libraries are required for example for radionuclide identification programs such as the WESPA (web spectrum analyser) module in Nucleonica. The libraries can be created using a range of commercial software, but usually the data (which includes nuclide, energies, emission probabilities, T1/2, etc.) has to be entered by hand. Also the underlying databases may not be up to date with the most recent nuclear data. Using the Gamma Library application in Nucleonica for this purpose makes life easier.

Gamma Spectrum Generator (GSG): To address these growing demands in gamma spectrometry, an interactive web-accessible simulation tool has been developed for use in Nucleonica. The simulator presents an efficient visual teaching aid that is especially useful in training facilities, which have restrictions on the use of radioactive substances, or when sources of special interest (e.g. spent fuel, enriched U, weapon grade Pu or other highly radiotoxic materials) are not readily available. The module is setup such that the user can run the program immediately through a simple "one-click" calculation with default parameters. This "one-click" calculation simulates the spectrum, for example, for a 10 MBq Co60 g-source located at 25 cm distance from unshielded 3" x 3" NaI detector. A more advanced version of the application – the GSG Pro - is available to study the effects of natural background and bremsstrahlung (e.g. for Sr-90).

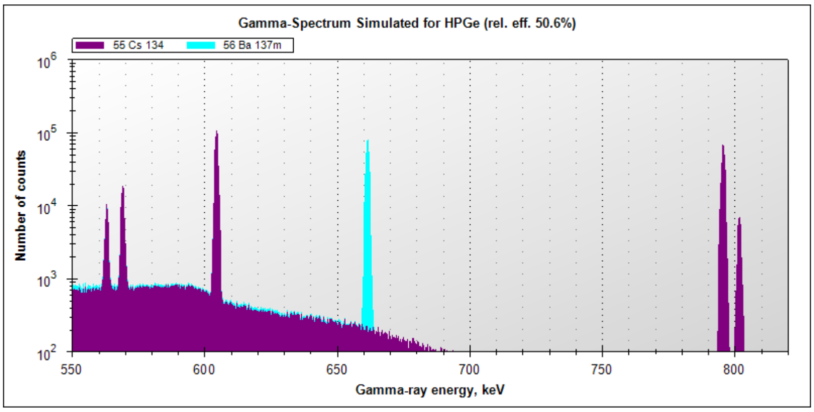

Figure 4: GSG simulation of the gamma spectrum of contamination at the Daiiichi plant, Fukushima. Contamination is almost entirely to cesium-137 and cesium -134

WESPA: (Web-based Spectrum Analyser) is an interactive peak-search based gamma spectrum analysis tool. Through an intuitive interface, it allows the user to assist in the identification process. One of the basic principles is the use of dedicated gamma libraries for nuclides to be expected in the sample. This simplifies the analysis process and allows for fast identification of the nuclides concerned. The specific nuclide libraries can be created with Nucleonica's library creation tool. In addition, a general library can be used where there is no information on the sample content available. WESPA can process spectral files with the IAEA *.spe format directly. Other formats need to be first converted using the Cambio file converter application in Nucleonica. The program includes peak search, energy, efficiency, and FWHM calibration. Energy dependent efficiencies are calculated from the detector supplier data and information about source matrix and absorbers.

Cambio File Convertor: Cambio was developed in response to a need of nuclear emergency response analysts everywhere to be able to quickly read the data from any of a widely growing number of formats used by both commercial and government detector systems worldwide. As the number of manufacturers of nuclear detection instrumentation grows, so does the number of data formats that must be able to be read by emergency analysts. Manufacturers of instrumentation often need to create new and more complex versions of their own formats as technology advances and as new user requirements lead to new, more sophisticated instruments.
File Conversion in 4 steps: The file conversion is completed as follows: 1) Select a file to be uploaded for conversion. The full filename of the file to be uploaded is shown. After selection of the appropriate input file, this can then be converted to one of the eight general file formats; 2) Select one of eight target file formats from the drop-down menu. The eight

conversion formats are: IaeaSpe, N42Xml, OrtecChn, DetectiveSpc, IdentiiFinderSpc, Gr130Dat, Gr135Dat, and GadrasPcf; 3) Start the conversion; If the input file is converted to the IaeaSpe or N42Xml formats, then a graph of the data can be viewed in the *Spectrum* tab; 4) Download the converted file.

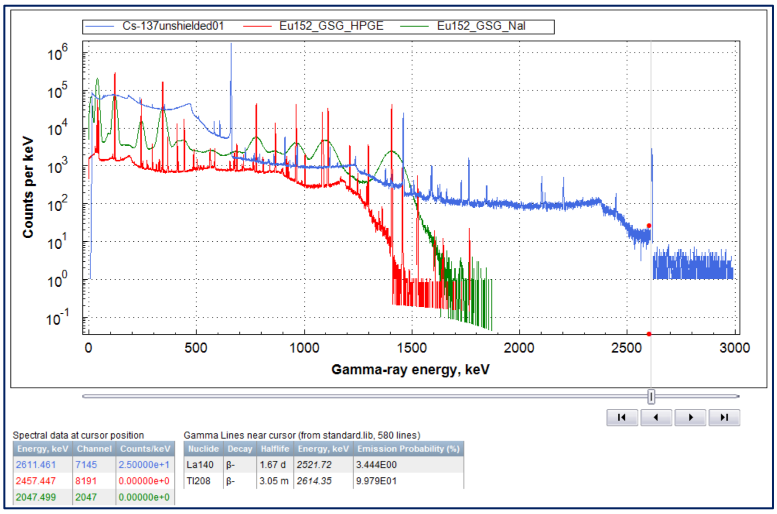

Figure 5: Multiple spectra comparison using Cambio

Nucleonica Scripting: The Nucleonica scripting is an object oriented language which is based on the physically intuitive classes, methods and properties. Through the script interface the user has access to the main Nucleonica applications and nuclear data. By combining results from multiple Nucleonica applications and nuclear data, users can go beyond the conventional single application approach for solving their specific experimental tasks and problems. Nucleonica applications are designed to be very user-friendly, intuitive, and require a minimum of learning time. For users, who prefer a more "hands on" approach, Nucleonica provides this with its scripting module. Scripting refers to a programming task, in which pre-existing components or applications are connected to accomplish a new task. In accordance with this definition, the Nucleonica scripting gives the user a powerful programming interface through which he/she can access basic nuclear data and run all the Nucleonica applications.

3.1 Verification, Validation and Testing

For the physical scientist, it is primarily of importance to know if the calculated results are "correct" – i.e. to what extent the results agree with experiment and/or other computer programs. Validation assures that the results agree with experiments and/or other programs. Verification aims at checking that the product has been built according to the requirements and design specifications. Testing is the process by which bugs and error are eliminated. In this context the Nucleonica modules are undergoing continuous development based on user-feedback through questions, remarks, and suggestions, for example, in the Nucleonica Forum. In particular there are two main questions of interest: How reliable is the nuclear data in Nucleonica? How reliable are the results from the calculation modules? Detailed information is given in the Nucleonica wiki [2].

4 EDUCATION AND TRAINING IN NUCLEAR SCIENCE

If one is going to deliver the long term goal of sustainable nuclear energy, it will be necessary to have an adequate resource of well-educated and trained young professionals coming into the field, whilst retaining the expertise and competencies. The Nucleonica

nuclear science portal is an innovative professional and technical resource for hands-on nuclear science education, for the nuclear industry. The Nucleonica team is very much involved in training [3]. The courses are aimed at persons who provide technical support (measurements, interpreting results, drawing conclusions, making recommendations) for the actions in response to environmental radioactivity issues, nuclear security, nuclear decommissioning, etc. A unique feature of the courses is the emphasis on interactive and hands-on learning through the use of the Nucleonica applications - a suite of powerful and versatile web-based applications. One of the main aims of the courses is to contribute to establishing a safety culture among the scientists and especially the younger generation of scientists. This safety culture is a necessary prerequisite to a general acceptance of nuclear energy worldwide. This international safety concern may be summarised as… “a nuclear accident anywhere is an accident everywhere”.

4.1 Post-graduate research using Nucleonica

Nucleonica is currently being used by a number of students for post-graduate research. Some examples of such studies are:

1. Ph.D study of nuclear fuel cycles: The content is to calculate the material flow in already established nuclear fuel cycles calculated with different input data (burnup, tHM, enrichment, MOX composition, length of fuel cycle, load factor, etc). The main goal is to derive and compare the amount of HLW which is stored and/or disposed for different fuel cycles, normalized to the same energy production.

2. MPhil studies on modelling of atmospheric dispersion of radionuclide release from a research reactor. The reactor is a highly enriched uranium low power research reactor tank-in-pool closed core. The aim is to compute: a) activity inventories of important radionuclides in the reactor core; b) release fractions; and c) activity released (to the atmosphere).

3. Ph.D. studies medical physics: simulation of a HPGe detector used in the laboratory using the Gamma Spectrum Generator application.

4. Ph.D studies on Monte Carlo dosimetry calculations. Development of a general dosimetry and shielding application based on the CERN code GEANT4 for inclusion into Nucleonica. The approach is similar to the development of the Virtual Cloud Chamber. Charged particles as well as photons and neutrons are to be included.

5. MPhil studies on performance assessment of a borehole disposal facility for sealed radioactive sources. Various Nucleonica tools will be used for decay calculations, heat generation, gamma emission, neutron emission, external and internal radiotoxicities, etc.

Many of the technical problems arising in the course of these studies have been discussed on the Nucleonica Forum [4]. Finally, we hope to be able to host the final reports from these studies on the Nucleonica web portal.

4.2 The Karlsruhe Nuclide Chart

For education and training purposes, the Karlsruhe Nuclide Chart is an indispensable tool. For more than 50 years, the Karlsruhe Nuclide Chart has provided scientists and students

with structured, accurate information on the half-lives and decay modes of radionuclides, as well as the energies of emitted radiation. An important characteristic of the Chart is its great didactic value in education and training in the nuclear sciences. The new 8th Edition of the "Karlsruher Nuklidkarte" [5] contains new and updated radioactive decay data on 737 nuclides not found in the previous (2006) edition. In total, nuclear data on 3847 experimentally observed ground states and isomers are presented. The new element names copernicium (symbol Cn element 112), flerovium (symbol Fl, element 114) and livermorium (symbol Lv, element 116) been introduced.

4.3 Nucleonica for Smartphones – M-Learning

Due to the rise in popularity of smartphones such as the Apple iPhone and the Samsung Galaxy, and the gradual evolution of e(lectronic)-learning through b(lended)-learning to now m(mobile)-learning, we have optimised many of the Nucleonica applications for used on such hand-held devices. This is of interest not only to students and a younger generation but also to to field workers and on mobile laboratories.

Figure 6: Nucleonica on smartphones: evolution from e-learning to m(obile)- learning

5 KNOWLEDGE MANAGEMENT

In this section, the Nucleonica web portal is considered from a knowledge management perspective. Of importance in this context is the "know-how" capture and transfer within organisations. One of the key issues here is how to extract the tacit knowledge from employees before they retire or leave an organisation and pass this on to a new generation of employees. Nonaka and Takeuchi [6] have proposed a model for organizational knowledge creation and transfer which is probably the most widely cited theory in knowledge management today.

6.1 Nucleonica's Knowledge Objects and the Knowledge Spiral

Nucleonica is based on a number of "knowledge objects" [7] ranging from the actual scientific applications to the forum and the wiki. In contrast to conventional paper-based documents, these are "electronic" knowledge objects (EKOs). The aim here is to produce high quality information resources which are easily accessible to any user. In the context of Nonaka's knowledge spiral and the SECI model, these EKOs are aimed at supporting and enhancing the knowledge creation, transfer, and dissemination processes. In this section, these EKOs are described in more detail. The Nucleonica nuclear science portal can be used as a

platform for organisational knowledge management in the nuclear domain. Nucleonica's "knowledge objects" are fully consistent with Nonaka's knowledge management theory and can be used for a technical implementation of the SECI model for knowledge socialisation, externalisation, combination and internalisation.

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